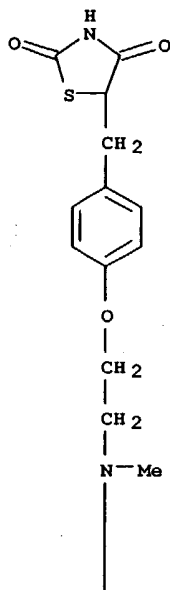
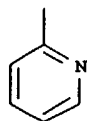


Registry Number: 122320-73-4

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Formula: C<sub>18</sub> H<sub>19</sub> N<sub>3</sub> O<sub>3</sub> S

CA Index Name: 2,4-Thiazolidinedione, 5-[[4-[2-(methyl-2-pyridinylamino)ethoxy]phenyl]methyl]- (9CI)

Other Names: 5-[4-[2-(N-Methyl-N-(2-pyridyl)amino)ethoxy]benzyl]thiazolidine-2,4-dione; BRL 49653; Rosiglitazone

-- Properties --

Property	Calculated Value	Condition	Note
Bioconc. Factor	1	pH 1	(1) ACD
Bioconc. Factor	1	pH 4	(1) ACD
Bioconc. Factor	7.30	pH 7	(1) ACD
Bioconc. Factor	1.11	pH 8	(1) ACD
Bioconc. Factor	1	pH 10	(1) ACD
Boiling Point	585.0±35.0 °C	Press: 760.0 Torr	(1) ACD
Enthalpy of Vap.	87.40±3.0 kJ/mol		(1) ACD
Flash Point	307.6±46.7 °C		(1) ACD
H acceptors	6		(1) ACD
H donors	1		(1) ACD
Koc	1	pH 1	(1) ACD

Koc	2.03	pH 4	(1) ACD
Koc	82.7	pH 7	(1) ACD
Koc	12.5	pH 8	(1) ACD
Koc	1	pH 10	(1) ACD
logD	-1.43	pH 1	(1) ACD
logD	0.10	pH 4	(1) ACD
logD	1.71	pH 7	(1) ACD
logD	0.89	pH 8	(1) ACD
logD	-0.96	pH 10	(1) ACD
logP	2.560±0.785		(1) ACD
Molar Solubility	Soluble	pH 1	(1) ACD
Molar Solubility	Slightly Soluble	pH 4	(1) ACD
Molar Solubility	Sparingly Soluble	pH 7	(1) ACD
Molar Solubility	Sparingly Soluble	pH 8	(1) ACD
Molar Solubility	Soluble	pH 10	(1) ACD
Molecular Weight	357.43		(1) ACD
pKa	6.34±0.50	Most Acidic	(1) ACD
pKa	6.48±0.12	Most Basic	(1) ACD
Vapor Pressure	1.14E-13 Torr	Temp: 25.0 °C	(1) ACD

Notes:

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 (© 1994-2004 ACD)

-- Resources --

References: ~832

STN Files: CAPLUS, ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CASREACT, CBNB, CEN, CHEMCATS, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, IPA, MEDLINE, MRCK, PHAR, PROMT, RTECS, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL

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